

Functionalized Cage Compounds: Computed NMR Shifts and Their Applications

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NMR spectra have been of a considerable importance also in elucidation of structural aspects of cage compounds. Computations can help in the task and enhance the observed information. In particular, *ab initio* computations of the NMR shielding tensors have recently been introduced, especially the Gauge-Independent Atomic Orbital (GIAO) method. In this contribution the relative NMR shifts are computed for selected cage compounds at several *ab initio* Hartree-Fock (HF) SCF levels using the GIAO approach. In a class of monoketo and diketo derivatives the error in the computed differences of the ^{13}C NMR shifts is only a few ppm at the HF/3-21G, HF/6-31G*, and HF/6-31+G(d,p) levels. A similar result is found for the computed relative ^{13}C NMR shift of C_{60} compared to benzene. Related results are also reported for fluorinated cages like $\text{C}_{60}\text{F}_{16}$ and $\text{C}_{60}\text{F}_{18}$ (^{19}F NMR shifts relative to C_{60}F_2). The results show applicability of the computations in some situations but also point out a need for still higher computational levels in other cases.